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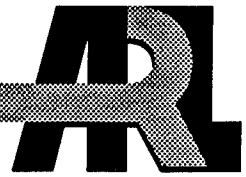
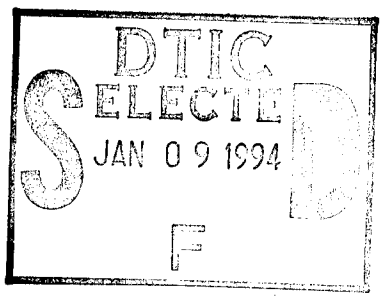


Ram Accelerator Performance Calculations Using a Modified Version of the NASA CET89 Equilibrium Chemistry Code

Federico Liberatore

ARL-TR-647

December 1994



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The equilibrium chemistry code, CET89, is modified to calculate the performance of ram projectiles using 1-D control volume derived governing equations. The modified program is capable of calculating the projectile thrust and chemical energy release as functions of projectile velocity. This information is then used to calculate the distance vs. time trace of a projectile traveling through an accelerator barrel. The modified program retains the full use of the thermodynamic database of the original code thus permitting performance calculations for a wide range of reactant mixtures.

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NOMENCLATURE

a	sound speed
b_1-b_7	polynomial coefficients from CET89 thermodynamic library
A	control volume cross-sectional area
C_v	fluid constant volume specific heat
C_p	fluid constant pressure specific heat
F	thrust force exerted by control volume on the projectile
h	sensible enthalpy
H	assigned enthalpy
ΔH_f^0	enthalpy of formation
M	Mach number = $\frac{U}{a}$
m	projectile mass
P	fluid pressure
Δq	change in enthalpy of formation
R	ideal gas constant
R_u	universal gas constant
S	fluid entropy
T	fluid temperature
U	fluid velocity
v	specific volume = $\frac{1}{\rho}$
x	projectile axial position
$\frac{dx}{dt}$	projectile velocity
$\frac{d^2x}{dt^2}$	projectile acceleration

NOMENCLATURE (continued)

GREEK SYMBOLS

γ	ratio of $\frac{C_p}{C_v}$
ρ	fluid density

SUPERSCRIPTS

'	beginning of next time interval

SUBSCRIPTS

0	reference temperature
1	control volume entrance plane
2	control volume exit plane

1. INTRODUCTION

1.1 **GENERAL BACKGROUND.** The successful operation of a ram accelerator projectile can be described as the proper matching of projectile speed and geometry to the available gas mixture, or vice-versa. The temperature rise across shock waves or boundary layers created by the geometry will eventually ignite the surrounding mixture. The amount of energy release and the location of the release around the body are what the projectile analyst must be concerned with. The combination of too high an energy release too far forward on the body will result in a pressure gradient that cannot be attained by attached oblique shocks and will cause the formation and upstream propagation of a normal shock/detonation wave. Too low an energy release too far aft on the body will result in little or no thrust.

The a priori prediction of the performance of a ram accelerator projectile can quickly turn into a formidable challenge if one cannot make use of simplifying assumptions. Unfortunately, the University of Washington (UW) derived geometry/gas mixture combination, currently the focus of attention at the major ram acceleration research centers, is one that defies simplifying assumptions. The geometry of the projectile features an axisymmetric right circular nose-cone, an axisymmetric truncated right circular cone aft-body, and four (or five) equally spaced fins which have swept back leading edges. The fins, in particular, give the flow field a strong three-dimensional character and the shocks emanating from the fin leading edges play a strong role in igniting the gas mixture. Given these circumstances, performance calculations which ignore fin effects and assume an axisymmetric flow field are, at best, approximate. The gas mixtures that have been used to date also contribute to the analytical complexity of the problem. The methane, oxygen, and nitrogen mixtures that have been used can be described as heavily diluted (with nitrogen) and very fuel rich which results in a reaction that, in comparison to an undiluted stoichiometric mixture, is relatively slow and mild. If equilibrium chemistry is used as a simplifying assumption, validation by comparison with finite rate kinetics chemistry should be made.

The ram accelerator analyst has to make judgements concerning the complexity of the fluid dynamics and the complexity of the chemistry for a given calculation. The ability to pare down the complexity of a calculation allows, given fixed computer resources, more calculations of a less detailed nature to be performed. If these less detailed calculations are "sufficiently" accurate, the ability to generate many calculations makes it possible to undertake proper

projectile/gas mixture design studies. The assessment that the approximate calculations are good enough has to be made through comparison with a more detailed and computationally intensive method such as computational fluid dynamics (CFD). In this case, CFD would serve as the first reality check for a given design and could be used to determine the validity of any simplifying assumptions that were used.

The ability to perform CFD calculations for high-speed, chemically reacting flow fields found in ram accelerators has been demonstrated by the Army Research Laboratory (ARL) (Nusca 1993), Amtec Engineering (Soetrisno, Imlay, and Roberts 1992), the Air Force Armament Directorate (Sinha et al. 1992), the Naval Research Laboratory (NRL) (Li et al. 1993a; Li et al. 1993b), and probably others (considering the similarities between ram accelerators and ramjet/scramjet propulsion). One-dimensional (1-D) control volume based methods have been demonstrated by UW (Knowlen and Bruckner 1991; Bruckner, Hertzberg, and Knowlen 1990; Bruckner et al. 1991), the Air Force Armament Directorate (Rolader and Drabczuk 1993), ISL and others (Brouillette et al. 1993). CFD solutions are dependant on projectile geometry but control volume solutions are independent of projectile geometry. Geometry-dependent approximate calculations have been made (Rom and Avital 1992), but not by any of the major ram accelerator research centers. The scramjet community has employed geometry-dependent approximate techniques for years so it appears that the ram community should have an interest in developing these kinds of tools for design purposes.

In light of all the aforementioned caveats, attention will now be focused on the derivation of governing equations for the 1-D control volume, equilibrium chemistry ram accelerator. Following that will be a discussion about how the fluid dynamic equations were incorporated into the NASA Lewis CET89 code. The NASA Lewis CET89 code was used as the equilibrium chemistry engine and thermodynamic database, thus resulting in an analytical model that combines the very simplest fluid dynamics with sophisticated chemistry. Documentation of the CET89 code is contained within NASA SP-273 (Gordon and McBride 1976) which is referred to frequently in this report. A detailed listing of the thermodynamic database used in NASA SP-273 is contained within NASA TM-4513 (McBride, Gordon, and Reno 1993)

1.2 **GOVERNING EQUATIONS.** Figure 1 shows the control volume around a HIRAM (Hybrid Inbore RAM) projectile that is travelling inside a gun tube.

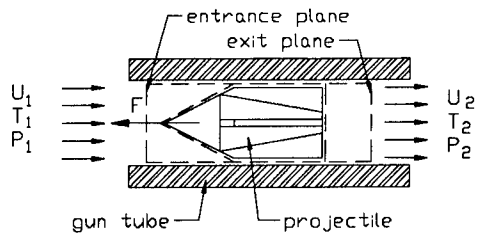

Figure 1: 1-D control volume used for ram projectile analysis.

The 1-D governing equations are:

$$\rho_1 U_1 = \rho_2 U_2 \qquad \text{continuity} \qquad (1)$$

$$P_1 + \rho_1 U_1^2 + \frac{F}{A} = P_2 + \rho_2 U_2^2 \qquad \text{momentum} \qquad (2)$$

$$H_1 + \frac{1}{2} U_1^2 = H_2 + \frac{1}{2} U_2^2 \qquad \text{energy} \qquad (3)$$

The assigned enthalpy at a given temperature, H, is defined as the enthalpy of formation at a reference temperature (in this case, the reference temperature is 298.15 K) plus the change in sensible enthalpy between the given temperature and the reference state.

$$H = \Delta H_f^0 + \left(h - h^0\right) \qquad (4)$$

The set of governing equations for the 1-D ram accelerator are identical to those that govern 1-D detonation waves except for the presence of the thrust parameter, $\frac{F}{A}$. Analysis of the 1-D ram accelerator is patterned after the analysis of detonation waves, which has been covered by various authors (Williams 1985 and Kuo 1986, to name just two). The analogy to 1-D detonation waves has to be emphasized strongly because the geometry of the projectile does not get factored into the final solution. This, along with the assumptions of 1-D flow in and 1-D flow out simplifies the whole ram process (oblique shocks, reflections, etc...) to a

planar phenomenon. The net result of all the simplifying assumptions is shown schematically in Figure 2.

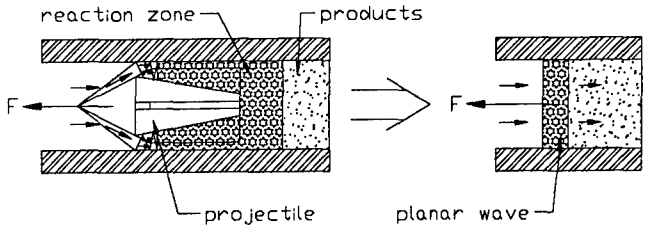

Figure 2: Schematic representation of the 1-D flow, equilibrium chemistry analogy to the ram acceleration process.

The ram projectile can be thought of as a 1-D detonation wave travelling through the gun tube. If the velocity of the projectile differs from the Chapman-Jouget detonation velocity, then the thrust, F, will be something other than zero.

Dividing through Equation (2) by P_1, rearranging, and using the continuity relation gives the following:

$$\frac{P_2}{P_1} - \left(\frac{F}{AP_1} + 1\right) = \frac{P_2}{P_1}\rho_2 \frac{U_2^2}{P_2}\left(\frac{\rho_2}{\rho_1} - 1\right) \qquad (5)$$

The assumption is made that the gas is ideal in behavior. This allows one to take advantage of the ideal equation of state and the sound speed relation in an ideal gas.

$$P\left(\frac{1}{\rho}\right) = RT = \left(\frac{1}{\gamma}\right)a^2 \qquad (6)$$

Equation (6) is substituted into Equation (5), and $\frac{U_2}{a_2}$ is replaced with M_2, the Mach number.

$$\frac{P_2}{P_1} = \frac{1}{1 - \gamma_2 M_2^2\left(\frac{\rho_2}{\rho_1} - 1\right)}\left(\frac{F}{AP_1} + 1\right) \qquad (7)$$

The Mach number in the exit plane is assumed to be equal to 1. This is the same assumption used in the analysis of detonation waves and, in the ram accelerator case, is referred to as the

"thermally choked mode." It seems arbitrary, but in the case of detonation waves, it is justified when it is shown that $M_2 = 1$ corresponds to a minimization of entropy and that experimentally observed detonations are well predicted when this assumption is made. $M_2 = 1$ defines the Chapman-Jouget condition in detonation waves, so the ram accelerator case amounts to calculating the Chapman Jouget points for $\frac{F}{AP_1} \neq 0$.

Substitution of Equation (4) into Equation (3) shows that the energy that drives the process comes from the release of chemical energy and this energy is equivalent to the change in enthalpy of formation from reactants to products.

$$\Delta q = \left(\Delta H_f^0\right)_1 - \left(\Delta H_f^0\right)_2 \qquad (8)$$

Classical textbook analyses often make the assumption of a calorically perfect gas. This allows C_p and γ to be treated as constant with temperature and, along with the ideal equation of state, let one combine the continuity, momentum, and energy equations so the thermodynamic end state, $\frac{P_2}{P_1}$, can be calculated as an explicit function of $\frac{\rho_2}{\rho_1}$ with $\frac{F}{A\,P_1}$ and $\Delta q\left(\frac{1}{(C_pT)_1}\right)$ handled as parameters that one can just plug in values for. The solution described in this discussion does not make the assumption of a calorically perfect gas, but the use of the dimensionless variable, $\Delta q\left(\frac{1}{(C_pT)_1}\right)$, is retained to be used as a principal indicator of the strength of the chemical reaction. The consequence of not assuming a calorically perfect gas is that an iterative solution scheme is required to arrive at the final end state of the reaction. This is discussed in the following section.

1.3 **MODIFICATIONS TO CET89 SOLUTION TECHNIQUE.** The NASA-Lewis CET89 code calculates the velocity and thermodynamic properties of Chapman-Jouget detonations. The near identical nature of the ram accelerator governing equations suggested the modification of the existing code and the solution algorithms to permit the inclusion of the thrust coefficient, $\frac{F}{A\,P_1}$. Following the assumptions made in NASA SP-273, the two equations to solve are

$$\frac{P_1}{P_2} = \left(1 - \gamma_2 M_2^2 \left(\frac{\rho_2}{\rho_1} - 1\right)\right)\left(\frac{1}{1 + \frac{F}{AP_1}}\right) \tag{9}$$

$$H_2 = H_1 + \frac{1}{2} M_2^2 \gamma_2 \, R_2 T_2 \left(\left(\frac{\rho_2}{\rho_1}\right)^2 - 1\right) \tag{10}$$

which reduce to Equations (170) and (171) in NASA SP-273 when $\frac{F}{A\,P_1} = 0$ and $M_2 = 1$. The next important step in SP-273 is the set up of the iteration scheme used to arrive at the final state of the detonation process which is given by Equation (174) and Equation (175). These two equations are used to solve for two unknowns, $\Delta \ln\left(\frac{P_2}{P_1}\right)$ and $\Delta \ln\left(\frac{T_2}{T_1}\right)$, which are the corrections to guessed values of $\frac{P_2}{P_1}$ and $\frac{T_2}{T_1}$. The corrections are used to update the current values and iterations are carried out until the corrections are smaller than 0.5×10^{-4} or until eight iterations are made (which is considered to be the "no convergence" threshold). The coefficients and non-homogeneous terms are calculated using the current values of $\frac{P_2}{P_1}$ and $\frac{T_2}{T_1}$. Since Equation (10) above is identical to Equation (171) in SP-273 (M_2=1 is assumed from now on), no modifications are necessary to the coefficients in the iteration scheme. The coefficients for Equation (174) in SP-273 have to be modified to reflect the presence of $\frac{F}{AP_1}$ in Equation (9) above.

$$\frac{\partial}{\partial}\frac{\left(P'' - \frac{P_1}{P_2}\right)}{\left(\ln\frac{P_2}{P_1}\right)} = \frac{P_1}{P_2} + \frac{1}{1 + \frac{F}{AP_1}} \gamma_2 \frac{\rho_2}{\rho_1} \frac{\partial}{\partial}\left[\frac{ln(V)}{ln(P)}\right]_{T,2} \tag{11}$$

$$\frac{\partial}{\partial}\frac{\left(P'' - \frac{P_1}{P_2}\right)}{\left(\ln\frac{T_2}{T_1}\right)} = \frac{1}{1 + \frac{F}{AP_1}} \gamma_2 \frac{\rho_2}{\rho_1} \frac{\partial}{\partial}\left[\frac{ln(V)}{ln(T)}\right]_{P,2} \tag{12}$$

$$\frac{P_1}{P_2} - P'' = \frac{P_1}{P_2} - \left(1-\gamma_2\left(\frac{\rho_2}{\rho_1}-1\right)\right)\left(\frac{1}{1+\frac{F}{AP_1}}\right) \tag{13}$$

These reduce to, respectively, Equations (176), (177), and (178) in SP-273 when $\frac{F}{A P_1} = 0$. The variable P'' represents the right-hand side of Equation (9) and is used to determine if convergence has been achieved. Convergence occurs when $\frac{P_1}{P_2} - P'' = 0$.

Two more concerns need to be addressed before the modified iteration scheme can be used to calculate the thrust curve of a ram projectile. The first concern is that one can't just arbitrarily pick values of $\frac{F}{A P_1}$ and calculate a final state. $\frac{F}{A P_1}$ is bounded with no solutions existing above a maximum value, $\left[\frac{F}{AP_1}\right]_{max}$. The second concern is that there are actually two solutions (two possible final states) for each value of $\frac{F}{A P_1}$ below the maximum value. When $\frac{F}{A P_1} = 0$, this other end point is called the Chapman-Jouget (or strong) deflagration point. When viewing the end points of the Chapman-Jouget detonation and deflagration of a typical mixture in a plane defined by the dimensionless thermodynamic variables, $\frac{P_2}{P_1}$ and $\frac{v_2}{v_1}$, the end point of the detonation solution has $\frac{P_2}{P_1} \gg 1$ and $\frac{v_2}{v_1} \cong 0.5$, whereas the deflagration solution has $\frac{P_2}{P_1} \cong 0.5$ and $\frac{v_2}{v_1} \gg 1$ where $\left(\frac{P_2}{P_1}, \frac{v_2}{v_1}\right) = (1,1)$ represent the initial unreacted state. In most textbooks, the only other observation made about the strong deflagration solution is that it is never observed in reality so it is treated as a reject root. For the case where $\frac{F}{AP_1} \neq 0$, rejection of all the deflagration solutions cannot be justified that easily. With larger values of $\frac{F}{AP_1}$, the two roots move closer to one another until, at the point on the thrust curve where $\frac{F}{A P_1} = \left[\frac{F}{A P_1}\right]_{max}$, the two roots degenerate to just one solution. In $\left(\frac{P_2}{P_1}, \frac{v_2}{v_1}\right)$ coordinates, this happens along the line $\frac{v_2}{v_1}=1$ which defines all the detonation branch solutions as those where

$\frac{v_2}{v_1}$<1 and the deflagration branch solutions as those with $\frac{v_2}{v_1}$>1. The solutions form a line in the $\left(\frac{P_2}{P_1}, \frac{v_2}{v_1}\right)$ plane that connect the Chapman-Jouget detonation and deflagration points. The solution will be unrealistic at the Chapman-Jouget deflagration point and some undetermined portion of the solution near the Chapman-Jouget deflagration point will be unrealistic as well. It is presently unclear how to precisely define this region so the entire solution is shown in the program output.

1.4 **INCORPORATION OF DIMENSIONLESS ENERGY RELEASE CALCULATION ROUTINE TO CET89.** CET89 reads in thermodynamic data from its library in the form of polynomial coefficients. These polynomial coefficients (b_1 through b_7) are used to define C_p, H, and S. The enthalpy of formation, $\Delta H_f^{0,T=298}$, is not directly defined in terms of polynomial coefficients, but can be calculated using expressions for H and C_p. Equations (90) and (91) of SP-273 give the polynomial expressions for C_p and H.

$$C_p = R_u\left[b_1 + b_2T + b_3T^2 + b_4T^3 + b_5T^4\right] \tag{14}$$

$$H = R_u\left[b_1T + \frac{b_2}{2}T^2 + \frac{b_3}{3}T^3 + \frac{b_4}{4}T^4 + \frac{b_5}{5}T^5 + b_6\right] \tag{15}$$

The change in sensible enthalpy is expressible as an integration of C_p.

$$\left(h - h_0\right) = \int_{T_0}^{T} C_p\, dT \tag{16}$$

Equation (4) can be rearranged to allow the calculation of ΔH_f^0.

$$\Delta H_f^0 = H - \int_{T_0}^{T} C_p\, dT \tag{17}$$

Substituting the polynomial expressions into Equation (17) leads to the expression used to calculate ΔH_f^0 for each species in the reaction.

$$\Delta H_f^0 = H\left(T_0\right) = R_u\left[b_1T_0 + \frac{b_2}{2}T_0^2 + \frac{b_3}{3}T_0^3 + \frac{b_4}{4}T_0^4 + \frac{b_5}{5}T_0^5 + b_6\right] \tag{18}$$

The contribution of all the reactant and product species are summed to give the non-dimensional heat release parameter.

$$\Delta q\left(\frac{1}{(C_pT)_1}\right) = \left(\gamma_1 - 1\right)\left(\frac{1}{a_1^2}\right)\left[\left(\Delta H_f^0\right)_1 - \left(\Delta H_f^0\right)_2\right] \tag{19}$$

1.5 **DISTANCE vs. TIME CALCULATION.** The purpose of calculating all the points in the P-v plane where solutions of the governing equations exist is to generate a thrust curve that shows the relationship between the dimensionless thrust coefficient, $\frac{F}{A\,P_1}$, and velocity. This calculated relationship can then be used to predict the distance vs. time history of a projectile inside a ram accelerator.

The acceleration of a ram projectile, at any given time, can be expressed by the following:

$$\frac{d^2x}{dt^2} = \frac{F}{m} = \frac{F}{AP_1} P_1 \left(\frac{A}{m}\right). \tag{20}$$

The acceleration of the projectile is controlled by $\frac{F}{A\,P_1}$, which is a result of the mixture composition and is weakly influenced by fill pressure, P_1, and the ratio of control volume cross-sectional area to projectile mass, $\frac{A}{m}$. The instantaneous acceleration is then used to predict velocity and position at the start of the next time increment.

$$\left(\frac{dx}{dt}\right)' = \frac{dx}{dt} + \frac{d^2x}{dt^2}(\Delta t) \tag{21}$$

$$x' = x + \frac{dx}{dt}(\Delta t) + \frac{d^2x}{dt^2}(\Delta t)^2 \tag{22}$$

The calculations are stopped when the distance exceeds the length of the barrel. The projectile is assumed to have zero acceleration upon entry into the ram accelerator. If the velocity of the projectile exceeds the Chapman-Jouget detonation velocity, the thrust is assumed to be equal to zero. The range of velocities calculated for the thrust curves spans from the Chapman-Jouget deflagration velocity to the Chapman-Jouget detonation velocity. Any velocity outside of these two limits would result in a negative thrust. The conclusion one can draw from this is that 1-D control volume based theories do not predict the attainability of projectile velocities above the Chapman-Jouget detonation velocity. This is contrary to what has been demonstrated experimentally by UW, where projectiles have been accelerated to velocities exceeding 150% of the Chapman-Jouget detonation velocity (Chew et al. 1991). This disparity emphasizes the need, on the part of the analyst, to excercise caution when using a theory that radically simplifies the physics of a given problem. It appears reasonable to

conclude that velocities in excess of the Chapman-Jouget detonation velocity can be achieved, but not by something that approximates the 1-D, thermally choked mode of operation outlined in this report. Also shown experimentally by UW is a deviation from 1-D, thermally choked theory in the transdetonative regime which begins at approximately 90% of the Chapman-Jouget velocity (Knowlen et al. 1991). A means for predicting the onset of the transdetonative regime (and defining the limits of applicability of the 1-D thermally choked model) is not yet available.

2. DISCUSSION

2.1 **PROGRAM MODIFICATIONS.** The CET89 code was modified by the addition of subroutines DEFLEG, MAXF, TCURVE, and QCALC. Entry OUT1A was added to the subroutine OUT1. The method of controlling the execution of the program, using an input file with controlling logical variables and needed parameters, was unchanged.

2.2 **PROGRAM EXECUTION.** The computer equipment needed to run the modified CET89 code is as follows:

1) IBM PC compatible computer
2) 80386 CPU or better
3) 80387 coprocessor or equivalent
4) MS-DOS operating system. NOTE: The code will not run inside the MS-DOS window within the Windows operating system.

In addition to the above requirements, the user might have to deactivate extended or expanded memory managers if their presence is incompatible with the protected mode memory routines that are bound with the program.

The executable file, nasa.exe and the two library files, thermo.bin and trans.bin, need to be located in a directory called c:\ram_cet. The program needs to load library data before a calculation is made, and the libraries are assumed to exist in directory c:\ram_cet.

A calculation is run by entering the command c:> nasa FILENAME.in where FILENAME.in is the input file that contains reactant data, initial conditions, and calculation instructions. An example input file is listed in Appendix 1. The .in suffix is required for input files.

The output files that are generated by input file FILENAME.in are FILENAME.out, FILENAME.plt, and FILENAME.xvt. FILENAME.plt appears if the thrust curve option is selected. FILENAME.xvt appears if the distance vs. time option is chosen. When the thrust curve option is chosen, FILENAME.out is created but its contents consist mostly of text headers and program diagnostics.

2.3 **EXECUTING NEW CALCULATIONS.** Calculation options in CET89 are selected by setting logical variables equal to true (ex: DETN=T) in the INPT2 NAMELIST variable input list. This controls the flow path through the program. The new calculation options are selected in the same manner and additional controlling logical variables are included to accommodate them. The logical variables and their functions are:

DEFLG=T	Chapman-Jouget deflagration point calculation
FMAX=T	Maximum thrust point calculation
TCURV=T	Calculate thrust vs velocity
XVST=T	Calculate projectile distance vs time trace

Thrust vs. velocity data is needed prior to calculating projectile distance vs. time so, if XVST=T is selected, TCURV=T must also be selected. In essence, DEFLEG=T, FMAX=T, and TCURV=T are stand alone options, while XVST=T is an option within an option.

2.4 **HEAT RELEASE PARAMETER CALCULATION.** The new subroutine QCALC is used to calculate the dimensionless heat release parameter. It is called by the other new subroutines. A modification was made to the existing Chapman-Jouget detonation calculation subroutine, DETON, to include the calling of subroutine QCALC. The energy release throughout the speed range of the RAM process when $\frac{F}{AP_1} \neq 0$ is fully accounted for.

The CET89 code suppresses the print-out of a product when its mole fraction is $<5\times10^{-6}$. More product information can be viewed if the trace option is selected. In the interest of speed, the calculation performed within QCALC is based only on the products having mole fractions $>5\times10^{-6}$.

2.5 **DEFLAGRATION AND MAXIMUM THRUST CALCULATION.** The new subroutines, DEFLEG and MAXF, are patterned after and are very similar to the existing subroutine DETON. The output provided by the subroutines DEFLEG and MAXF are identical in nature to that provided by the existing subroutine DETON in that detailed information is provided for pre-reaction, post-reaction, and overall performance parameters.

The changes made to DETON to create DEFLEG were very minor in nature. DETON assumes an initial guess for final temperature of 3,800 K and pressure ratio of 15. The subroutine then iterates until converging on the final solution. DEFLEG is a calculation for

the deflagration branch root to the same equation solved in DETON. The initial guesses for temperature and pressure ratio are changed to 2,500 K and 0.45, respectively, to allow the iteration routine to converge on the Chapman-Jouget deflagration point. To date (after an admittedly brief experience with the new routine), this approach and the initial estimates of temperature and pressure have been found to be adequate.

More substantial changes were made to go from subroutine DETON to subroutine MAXF. In the *P-v* plane, the location of the maximum thrust point will occur along the line $\frac{v_2}{v_1} = 1$. Examination of Equation (10) will show that, at the maximum thrust point, $H_2 = H_1$. The iteration technique used in DETON, where two equations are used to come up with corrections for temperature and pressure, is unnecessary. The iteration scheme in subroutine MAXF makes use of the ability of the CET89 code to specify thermodynamic state in terms of the variables *H* and *P* (HP=T option). The enthalpy of the reactants is calculated and remains a fixed input in the iteration scheme. After this is done, the pressure ratio is varied until the required condition of $\frac{v_2}{v_1} = 1$ is satisfied.

The required input for both of these calculation options is the same as that required for the detonation calculation. After the controlling logical variable is set true and included as part of the INPT2 name list, a set of initial temperatures and pressures (26 each max) is supplied. The output for a given input file, FILENAME.in, appears in an output file called FILENAME.out.

2.6 **THRUST CURVE CALCULATION.** The thrust curve routine finds all the locations in the *P-v* plane that lie between the Chapman-Jouget detonation and deflagration points and prints simplified output in a form suitable for input into a plotting program so that the thrust curve can be shown graphically.

The subroutine first calculates the location of the maximum thrust point using the same technique that is in subroutine MAXF. The reason for this is that no solutions exist for $\frac{F}{A P_1} > \left[\frac{F}{A P_1}\right]_{max}$. Once this is accomplished, the value of $\left[\frac{F}{A P_1}\right]_{max}$ is used to determine the values of $\frac{F}{A P_1}$ that will be input as parameters into the root-finding equations. A total of 43 points are used to make up a thrust curve. These are divided up into 21 points on the

detonation branch, 21 points on the deflagration branch, and the maximum thrust point which divides them. $\frac{F}{A\,P_1}$ is increased from zero to a value of $0.98 \times \left[\frac{F}{A\,P_1}\right]_{max}$ to fill in all the points in the detonation branch with data being written to the output file at the end of each stepwise increment. The data for the maximum thrust point, having already been calculated, is then written out. The deflagration branch is now filled in with the value of $\frac{F}{A\,P_1}$ being decreased back down to zero.

The second point calculated corresponds to the Chapman-Jouget detonation point. The method used to calculate this point is identical to that used in subroutine DETON. The next point calculated is the first one that uses the modified root-finding equations with a non-zero value of $\frac{F}{A\,P_1}$. The initial estimates of pressure and temperature for this point are those of the previously calculated point. It is believed that this method will provide for well-conditioned calculations. Each value of $\frac{F}{AP_1}$ has two roots, and, for values near $\left[\frac{F}{AP_1}\right]_{max}$, these two roots can be relatively close to one another. To prevent the iteration routine from possibly jumping to the opposite branch, traps are set to catch the program if it jumps to the other side of $\frac{v_2}{v_1}=1$ and restart it at a point close to the maximum thrust point but on the correct side of $\frac{v_2}{v_1}=1$.

The twenty-third point calculated is the first point calculated that lies on the deflagration branch. The initial estimates used for this point are based on the temperature ratio and pressure ratio of the maximum thrust point with small (0.1) decrements to place it on the deflagration branch side of the *P-v* plane. To date, this technique, along with the traps to guard against jumping to the opposite branch, have worked well.

The input required for a thrust curve calculation is the same as is required for the detonation calculation, a listing of the mixture initial temperatures and pressures (up to 26 each). The output for an input file FILENAME.in appears in an output file FILENAME.plt. The output is in the form of columns of velocity, Mach number, thrust coefficient, heat release parameter, temperature ratio, pressure ration, and specific volume ratio. This makes it

possible to plot thrust vs. velocity to obtain the thrust curve or cross plot pressure vs. specific volume to generate the locus of solution points in the P-v plane.

2.7 **DISTANCE vs. TIME CALCULATION.** The calculation of distance vs. time is an option that is executed within the subroutine TCURVE. After the final point of a thrust curve is calculated, distance vs. time calculations are made if the XVST=T option has been specified. Up to 27 distance vs. time calculations can be made for every thrust curve. This is comprised of three possible entrance velocities, three barrel lengths, and three accelerator cross-sectional area to projectile mass, $\frac{A}{m}$, ratios.

The calculation is begun by interpolating through the thrust curve data and finding the thrust coefficient for the entrance velocity. This is used to calculate projectile distance and velocity at the end of the time interval Δt. The value of the time interval is set by the following equation.

$$\Delta t = \frac{L_{barrel}/U_{entrance}}{N} \tag{23}$$

The default value of N is 50, but a different value can be specified in the input file. The position and velocity at the end of the time period become the initial values for the next time interval. This is repeated until the distance travelled exceeds the length of the barrel. If an initial velocity outside of the range of the thrust curve is specified, the calculation is not performed and the user is notified about the problem. If, in the course of the calculation, the projectile should get accelerated to a velocity faster than the Chapman-Jouget detonation speed, the thrust coefficient is set equal to zero and no further acceleration occurs.

The distance vs. time calculation is selected by setting XVST=T and by specifying the needed additional parameters in the INPT2 namelist along with the items required for a thrust curve calculation. The needed additional parameters are:

entrance velocity	$\left[\frac{m}{sec}\right]$	UENTR=1,2,3
$\frac{A}{m}$	$\left[\frac{m^2}{kg}\right]$	AMRAT=1,2,3
barrel length	$[m]$	BRLEN=1,2,3
time step intervals (optional)		NTINC= X (default=50)

The output generated from data in input file FILENAME.in appears in output file FILENAME.xvt. The output that is generated is organized in columns making it possible to quickly edit so than it can be used as the input to a plotting program. The data that appears in the output file is distance, time, velocity, and thrust coefficient.

2.8 **OTHER MODIFICATIONS.** Entry OUT1A was added to subroutine OUT1 in order to print out the precise pre-reaction mixture compositions and make it part of the output file. This is an issue if one specifies the reactant species as F(uel) and O(xidizer) and uses the options OF, FA, PHI, or EQRAT to define the reactant composition. In this case, what is calculated differs from what is shown on the input card according to the molar or mass coefficients for each species. It is intended that the calculation and print out of the pre-equilibrium composition eliminates the need to go back and hand calculate (using the values of PHI, OF, FA, and EQRAT that were used) to determine the reactant composition.

3. RESULTS

Figure 3 shows a sample thrust curve that was generated using data from the FILENAME.plt output file. The mixture composition and initial conditions correspond to the mixture used in the first successful live firing of the HIRAM facility at ARL. The locations of the Chapman-Jouget detonation point, Chapman-Jouget deflagration point, and maximum thrust point are marked. The domains of the detonation branch and the deflagration branch are also marked.

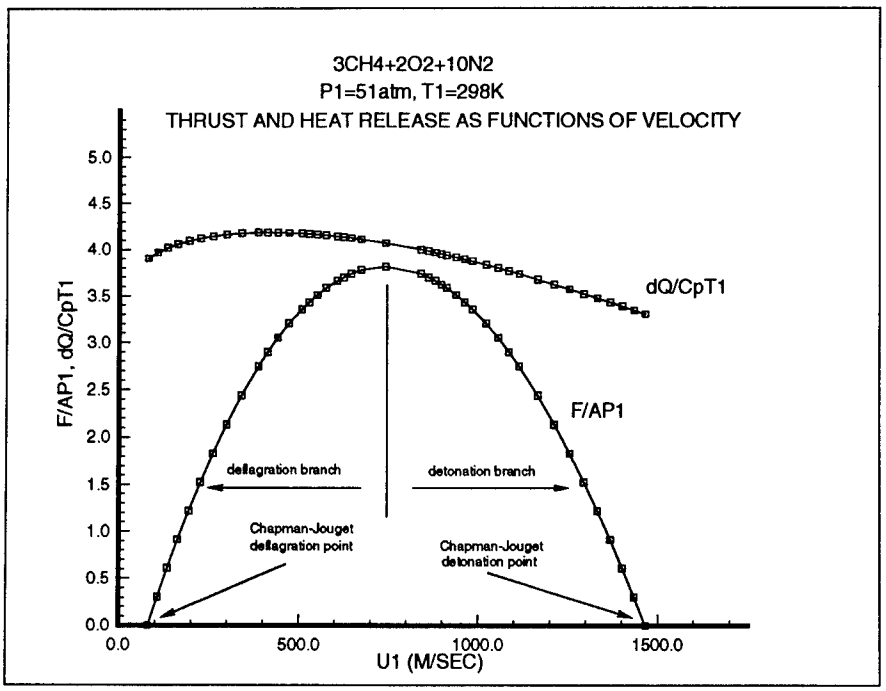

Figure 3: Thrust curve for the baseline HIRAM gas mixture.

It was stated previously that the 1-D control volume formulation reduces the projectile to a planar wave that is travelling through the gun barrel and that the Chapman-Jouget deflagration point is never observed in reality. Examination of the two end points of the thrust curve will show that the Chapman-Jouget detonation point is stable, whereas the Chapman-Jouget deflagration point is unstable. If a wave should be travelling at a speed lower than the detonation velocity, a positive force will be generated that will accelerate it, but if the wave should be travelling faster than the detonation velocity, a retarding force will be

generated instead (negative values of $\frac{F}{A P_1}$ were not calculated, but they do exist outside of the boundaries set by the Chapman-Jouget detonation and deflagration points). The opposite occurs at the Chapman-Jouget deflagration point, where the force induced when the wave is travelling at a velocity different than the deflagration velocity will move it further away from the deflagration point.

In addition to thrust vs. velocity, Figure 3 also shows the dimensionless energy release parameter as a function of velocity. Energy release does vary somewhat with velocity. Each calculated point corresponds to a different final pressure and temperature which results in a variation of the final mixture composition and enthalpy of formation of the final products.

Figure 4 shows the locus of thrust curve solution points in the *P-v* plane using data from the same FILENAME.plt output file that was used to generate Figure 3. The points that were marked in Figure 3 are also marked in Figure 4.

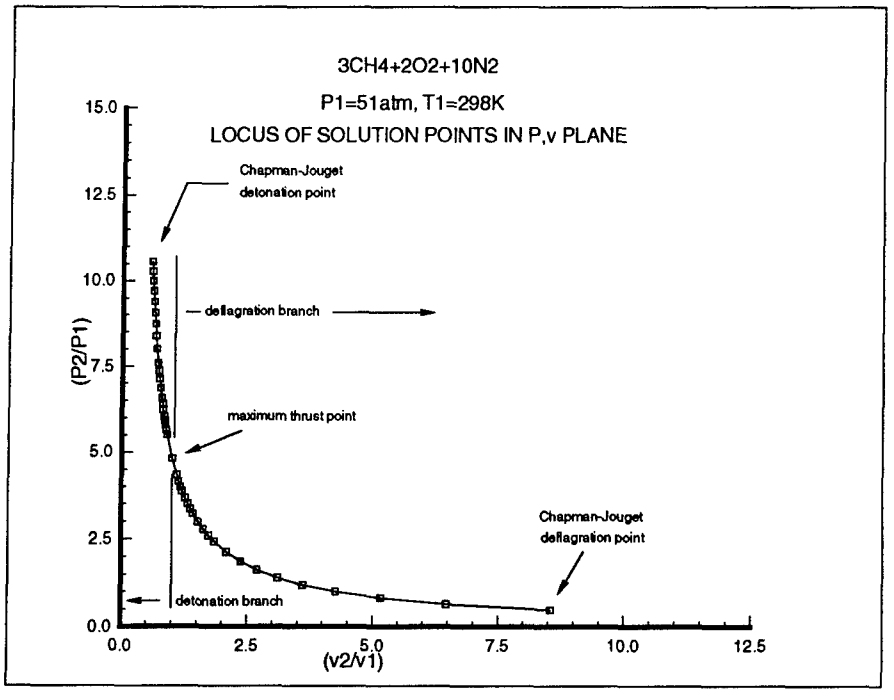

Figure 4: Thrust curve from Figure 3 in the thermodynamic plane.

Figure 5 shows a sample velocity vs. distance trace of a projectile that was generated using the thrust curve shown in Figure 3. Also plotted on Figure 5 is thrust coefficient vs.

distance. This shows graphically if the projectile is operating ineffectively and if a different reactant mixture should be considered.

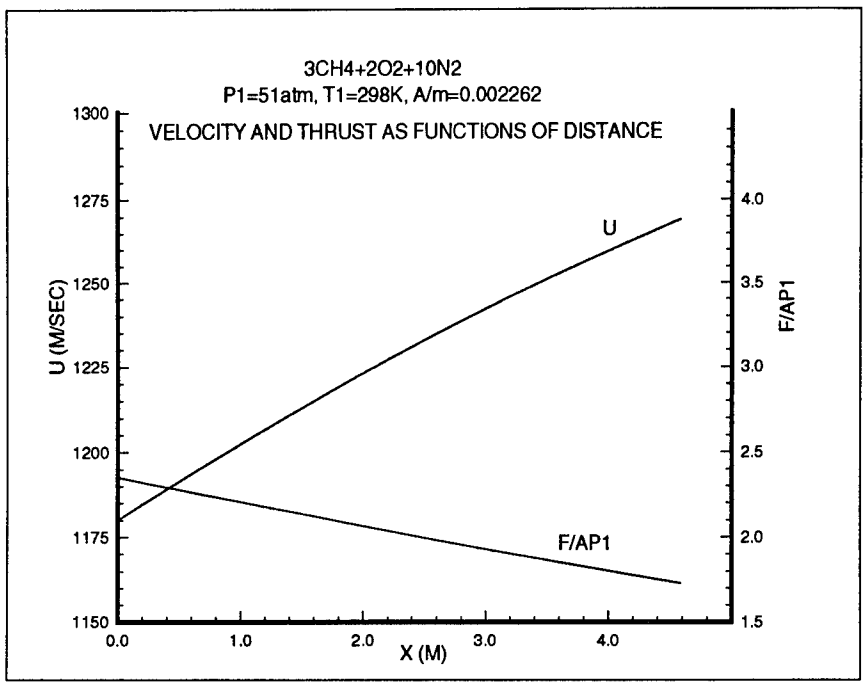

Figure 5: Sample distance vs. time calculation using the thrust curve from Figure 3.

Figures 6, 7, and 8 show, respectively, the same calculated results in Figures 3, 4, and 5, but for a different mixture at a different initial pressure. This particular mixture has never been tried in the HIRAM facility but has been used by UW. The UW mixture is slightly less fuel rich and significantly less diluted with nitrogen.

As expected, the less diluted mixture is more energetic and displays this increased energy release throughout the speed range of the ram acceleration process. The value of $\Delta q \frac{1}{\left(C_p T\right)_1}$ rises from 3.3 to 4.4 at the Chapman-Jouget detonation point and the difference throughout is approximately 1. The extra energy of the less dilute mixture results in an increase in the maximum thrust coefficient from 4.1 at 740 m/sec to 4.9 at 840 m/sec. The detonation velocity of the mixture also increased from 1,470 m/sec to 1,700 m/sec. The change in sound speed between the two mixtures is negligible (361 m/sec for the baseline mixture and

363 m/sec for the less dilute mixture) so the increased detonation speed is a result of only the greater energy release.

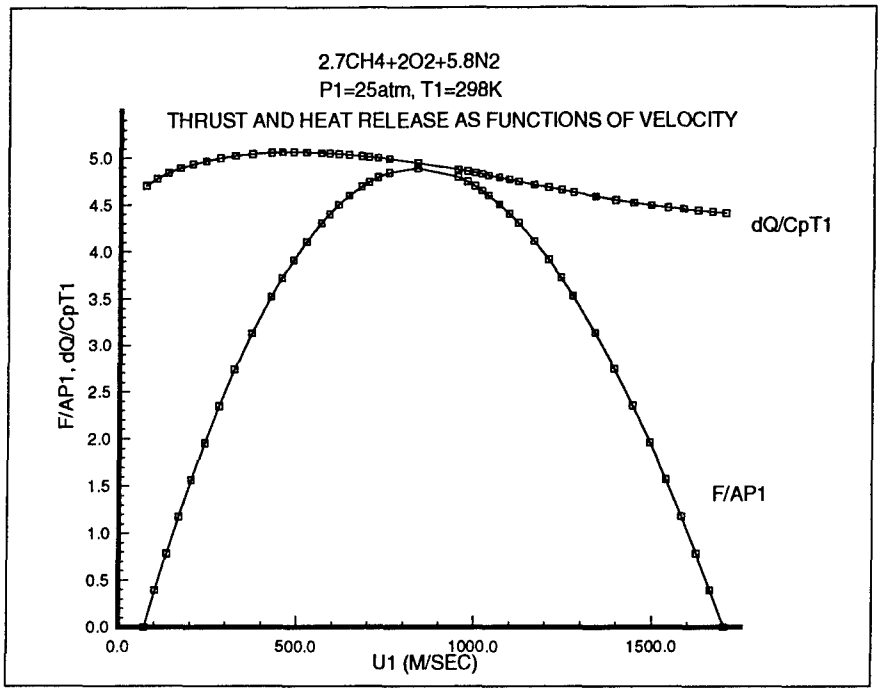

Figure 6: Thrust curve for a different gas mixture and fill pressure.

A comparison of the calculated thrust curve shown in Figure 6 with published thrust curves (Knowlen and Bruckner 1991; Rolader and Drabczuk 1993) is shown in Appendix 4. Figure 7 shows the thrust curve of Figure 6 plotted in P-v coordinates.

Another indication of the greater energy release of the less dilute mixture is the higher final pressure ratio achieved at the detonation point. Though not plotted, this is also accompanied with a higher final temperature ratio.

Figure 8 shows a distance vs time calculation using the thrust curve shown in Figure 6 with the same projectile parameters used in Figure 5 (entrance velocity = 1,180 m/sec, barrel length = 4.5 m, and cross-sectional area to mass ratio = 0.00226)

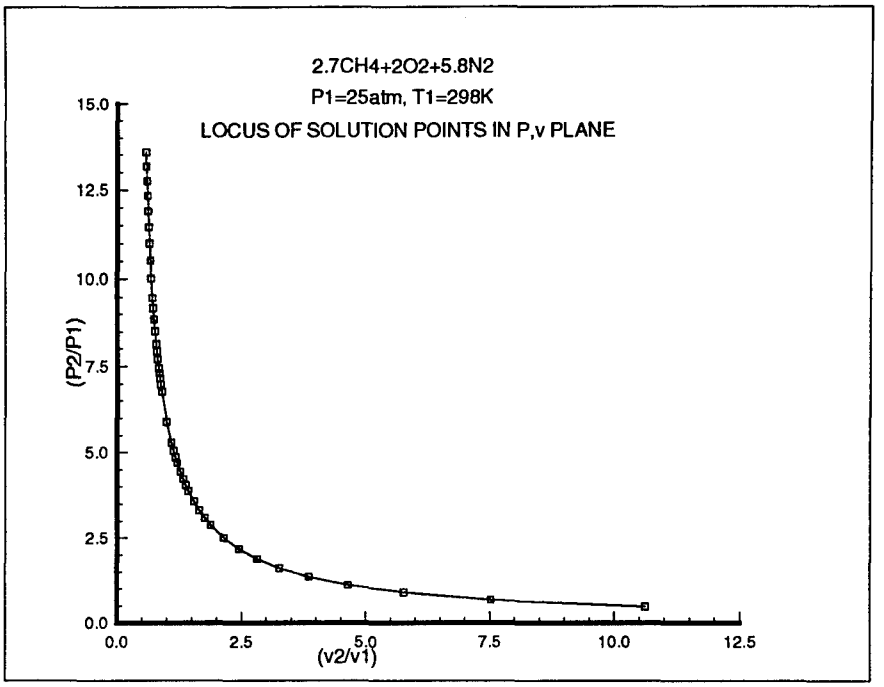

Figure 7: Thrust curve from Figure 6 in the thermodynamic plane.

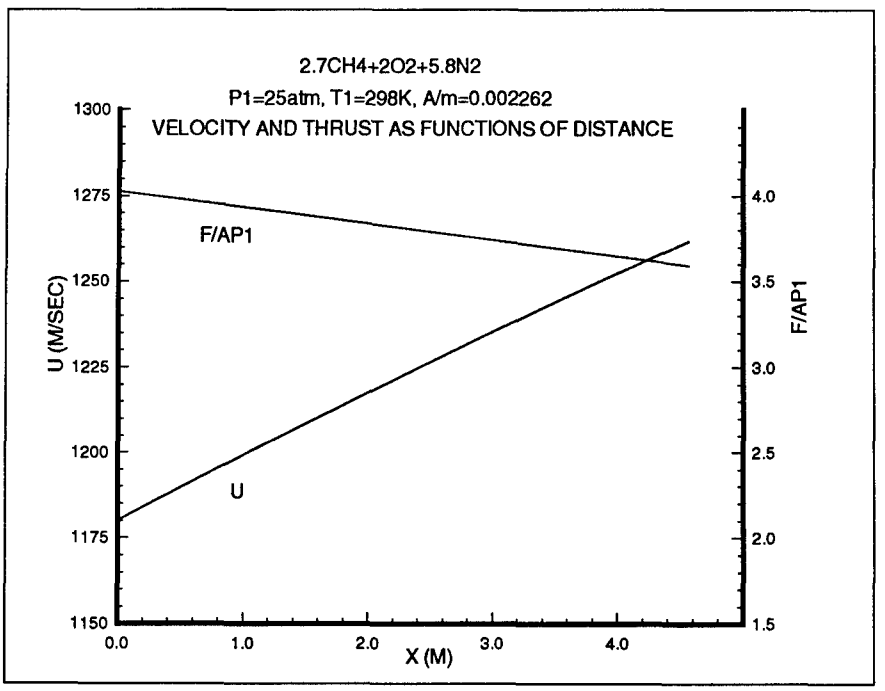

Figure 8: Distance vs. time calculation using the thrust curve from Figure 6.

Examination of Figure 8 and comparison with Figure 5 reveals some interesting results. Despite using only half the fill pressure, the exit velocity predicted for the UW mixture in Figure 8 is almost identical to that predicted in Figure 5 (1,262 m/sec vs. 1,269 m/sec). The reason for this is that the projectile in Figure 8 is operating at approximately double the thrust coefficient throughout the barrel compared to the HIRAM baseline mixture in Figure 5. The doubled thrust coefficient, $\frac{F}{A P_1}$, combined with half the fill pressure, P_1, result in the same thrust and exit velocity. Examination of the thrust curves in Figures 3 and 6 reveals that, for an entrance velocity of 1,180 m/sec, the ram process operates in a more effective portion of the thrust curve (closer to $\left[\frac{F}{AP_1}\right]_{max}$) using the UW mixture.

Caution has to be excercised if one is considering alternative mixtures to improve performance. The projectile's geometry will impose limits on how much heat can be released for a given Mach number. Control volume based theory cannot give this information. It has to be arrived at either through more sophisticated analysis or experimentation.

4. CONCLUSIONS

The modifications made to the CET89 program have resulted in the ability to calculate 1-D control volume ram accelerator thrust curves efficiently while also being able to access the CET89 thermodynamic library. This allows the possibility of analyzing the potential performance of a wide range of fuel mixtures. The most appropriate use of the program would be for preliminary studies of fuel mixtures. The performance of the projectile will be a function of dimensionless variables (M_1, $\Delta q \frac{1}{(C_p T)_1}$,...) and the modified CET89 code could be used to find mixtures that have the proper characteristics.

It is vital to understand that there are mixture properties important to projectile performance that are not calculated by the modified CET89 code. These are properties that are kinetic in nature, such as auto-ignition temperature, induction time, and reaction rate. The 1-D control volume equation does not allow for projectile geometry, so the analysis of a geometry and its interaction with the reactant mixture must be done with a more sophisticated theory, something that at least allows for area changes (a quasi 1-D theory) and finite rate chemistry.

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APPENDIX 1: Sample computer program input file.

The following is the input file that was read by the modified CET-89 code and generated the output used to create Figures 3, 4, and 5.

```
REACTANTS
C 1.     H 4.                    00       3.0     M0.0       G298.00  F
O 2.                             00       2.0     M0.0       G298.00  O
N 2.                             00       10.0    M0.0       G298.00  F

NAMELISTS
 &INPT2 TCURV=T,XVST=T,SIUNIT=T,ERATIO=T,
 T=298,P=51,MIX=3.0,NTINC=50,UENTR=1180.,BRLEN=4.5,AMRAT=0.002262 &END
```

The option TCURV=T selects the thrust curve calculation and this was used to provide the data for Figures 3 and 4 (see Appendix 2 for a listing of the data). The remaining inputs for a thrust curve calculation are identical to those needed for a detonation point calculation, reactant composition is specified and initial pressures and temperatures are given.

The XVST=T option selects the distance vs. time calculation. The additional parameters that need to be specified for a distance vs. time calculation are entrance velocity (UENTR=), barrel length (BRLEN=), tube cross-sectional area to projectile mass ratio (AMRAT=), and calculation time step interval (NTINC=). After a thrust curve calculation is completed (43 data points), distance vs. time calculations are made. The output of the data used to generate Figure 5 is shown in Appendix 3.

APPENDIX 2: Sample computer program output file for a thrust curve calculation.

```
    3.000 CH4  +  2.000 O2   + 10.000 N2
PRE-EQUIL COMPOSITION    0.008 CH4  +  0.005 O2   +  0.025 N2
   O/F=  0.1950    EQUIVALENCE RATIO= 3.0000
P1=  51.00 ATM : T1=  298.0 K
  U1        M1        F/AP1     Q/CpT1    T2/T1     P2/P1     RHO1/RHO2
   1466.3    4.0613    0.0000    3.3048    5.0655   10.5608    0.5787
   1435.0    3.9746    0.3051    3.3450    5.0153   10.2794    0.5871
   1402.5    3.8844    0.6103    3.3867    4.9649    9.9905    0.5963
   1368.6    3.7904    0.9154    3.4300    4.9139    9.6934    0.6065
   1333.0    3.6920    1.2206    3.4749    4.8622    9.3864    0.6179
   1295.6    3.5883    1.5257    3.5217    4.8096    9.0673    0.6307
   1255.8    3.4781    1.8308    3.5707    4.7556    8.7335    0.6453
   1213.1    3.3600    2.1360    3.6221    4.6997    8.3808    0.6623
   1166.7    3.2314    2.4411    3.6766    4.6413    8.0033    0.6824
   1115.2    3.0887    2.7463    3.7350    4.5791    7.5916    0.7070
   1086.8    3.0100    2.8988    3.7661    4.5460    7.3680    0.7217
   1056.1    2.9250    3.0514    3.7989    4.5111    7.1285    0.7386
   1022.3    2.8313    3.2040    3.8339    4.4736    6.8679    0.7585
    984.1    2.7256    3.3565    3.8718    4.4326    6.5770    0.7827
    962.7    2.6663    3.4328    3.8924    4.4101    6.4156    0.7973
    939.1    2.6009    3.5091    3.9144    4.3858    6.2388    0.8142
    912.4    2.5269    3.5854    3.9385    4.3588    6.0405    0.8344
    897.4    2.4854    3.6235    3.9515    4.3439    5.9299    0.8463
    880.8    2.4395    3.6617    3.9657    4.3277    5.8084    0.8600
    862.1    2.3876    3.6998    3.9812    4.3095    5.6715    0.8761
    839.9    2.3262    3.7380    3.9990    4.2884    5.5106    0.8962
    742.2    2.0555    3.8142    4.0691    4.1994    4.8142    1.0000
    673.8    1.8663    3.7761    4.1092    4.1408    4.3386    1.0913
    645.6    1.7881    3.7380    4.1234    4.1173    4.1446    1.1349
    624.0    1.7283    3.6998    4.1334    4.0996    3.9971    1.1710
    605.9    1.6781    3.6617    4.1411    4.0850    3.8741    1.2033
    575.6    1.5941    3.5854    4.1527    4.0607    3.6691    1.2621
    550.1    1.5235    3.5091    4.1610    4.0406    3.4981    1.3166
    527.7    1.4615    3.4328    4.1672    4.0231    3.3487    1.3689
    507.5    1.4056    3.3565    4.1719    4.0075    3.2147    1.4201
    471.8    1.3066    3.2040    4.1780    3.9799    2.9787    1.5216
    440.4    1.2197    3.0514    4.1809    3.9559    2.7731    1.6245
    412.1    1.1414    2.8988    4.1814    3.9342    2.5890    1.7307
    386.2    1.0697    2.7463    4.1799    3.9142    2.4210    1.8418
    339.6    0.9407    2.4411    4.1722    3.8777    2.1209    2.0844
    298.2    0.8258    2.1360    4.1592    3.8439    1.8559    2.3642
    260.5    0.7215    1.8308    4.1413    3.8116    1.6165    2.6956
    225.7    0.6252    1.5257    4.1187    3.7797    1.3968    3.0992
    193.3    0.5354    1.2206    4.0911    3.7471    1.1929    3.6058
    162.8    0.4509    0.9154    4.0577    3.7129    1.0019    4.2651
```

133.9	0.3710	0.6103	4.0173	3.6756	0.8218	5.1639
106.5	0.2948	0.3051	3.9677	3.6334	0.6510	6.4687
80.2	0.2220	0.0000	3.9049	3.5831	0.4883	8.5466

APPENDIX 3: Sample computer program output for a distance vs time calculation.

```
    3.000 CH4  +  2.000 O2   + 10.000 N2
PRE-EQUIL COMPOSITION    0.008 CH4  +  0.005 O2   +  0.025 N2
   O/F=  0.1950    EQUIVALENCE RATIO= 3.0000
 FILL PRES = 51.00 ATM,  FILL TEMP =298.00 K
 U0 = 1180.0 M/SEC,  ACCEL LEN =   4.50 M,  A/M =0.00226 M^2/KG
 X [M]     T [SEC]     U [M/SEC]  F/AP1
  0.0000   0.000000    1180.00    2.3538
  0.0901   0.000076    1182.10    2.3400
  0.1803   0.000153    1184.18    2.3263
  0.2707   0.000229    1186.26    2.3126
  0.3613   0.000305    1188.32    2.2991
  0.4520   0.000381    1190.37    2.2856
  0.5429   0.000458    1192.41    2.2722
  0.6339   0.000534    1194.43    2.2589
  0.7251   0.000610    1196.45    2.2456
  0.8164   0.000686    1198.45    2.2325
  0.9079   0.000763    1200.44    2.2194
  0.9995   0.000839    1202.42    2.2064
  1.0913   0.000915    1204.39    2.1935
  1.1832   0.000992    1206.34    2.1806
  1.2753   0.001068    1208.29    2.1678
  1.3675   0.001144    1210.22    2.1551
  1.4599   0.001220    1212.14    2.1425
  1.5524   0.001297    1214.05    2.1294
  1.6451   0.001373    1215.95    2.1158
  1.7379   0.001449    1217.83    2.1023
  1.8309   0.001525    1219.71    2.0889
  1.9240   0.001602    1221.57    2.0756
  2.0172   0.001678    1223.42    2.0624
  2.1106   0.001754    1225.26    2.0492
  2.2041   0.001831    1227.09    2.0362
  2.2978   0.001907    1228.90    2.0232
  2.3916   0.001983    1230.71    2.0103
  2.4855   0.002059    1232.50    1.9975
  2.5796   0.002136    1234.28    1.9847
  2.6738   0.002212    1236.05    1.9721
  2.7681   0.002288    1237.81    1.9595
  2.8626   0.002364    1239.55    1.9470
  2.9572   0.002441    1241.29    1.9346
  3.0520   0.002517    1243.01    1.9223
  3.1468   0.002593    1244.73    1.9100
  3.2418   0.002669    1246.43    1.8978
  3.3370   0.002746    1248.12    1.8857
  3.4322   0.002822    1249.80    1.8737
  3.5276   0.002898    1251.47    1.8618
```

3.6231	0.002975	1253.13	1.8499
3.7188	0.003051	1254.78	1.8381
3.8145	0.003127	1256.42	1.8261
3.9104	0.003203	1258.05	1.8136
4.0064	0.003280	1259.67	1.8012
4.1026	0.003356	1261.27	1.7889
4.1988	0.003432	1262.87	1.7766
4.2952	0.003508	1264.45	1.7645
4.3917	0.003585	1266.03	1.7524
4.4883	0.003661	1267.59	1.7404
4.5851	0.003737	1269.14	1.7285

NUMBER OF POINTS IN CURVE = 50

APPENDIX 4: Comparison of calculated thrust curve to published results.

Figure 9 shows a comparison of the thrust curve shown in Figure 6 of this report with thrust curves published by UW (Knowlen and Bruckner 1991) and by the Air Force Armament Directorate at Eglin AFB (Rolader and Drabczuk 1993). The UW and Eglin curves were reproduced with the aid of a digitizing tablet which was used to generate coordinate data. The UW and the Eglin plots, in their original forms, had thrust coefficient plotted against dimensionless velocities, Mach number in the Eglin case and $\frac{U}{U_{CJ}}$ in the UW case. The dimensionless velocity values read with the digitizer were then multiplied by, respectively, sound speed (363.4 m/sec) and Chapman-Jouget detonation velocity (1,701.4 m/sec) to make a direct comparison with the thrust curve calculated with the modified CET89 code. The agreement between the three curves is very good.

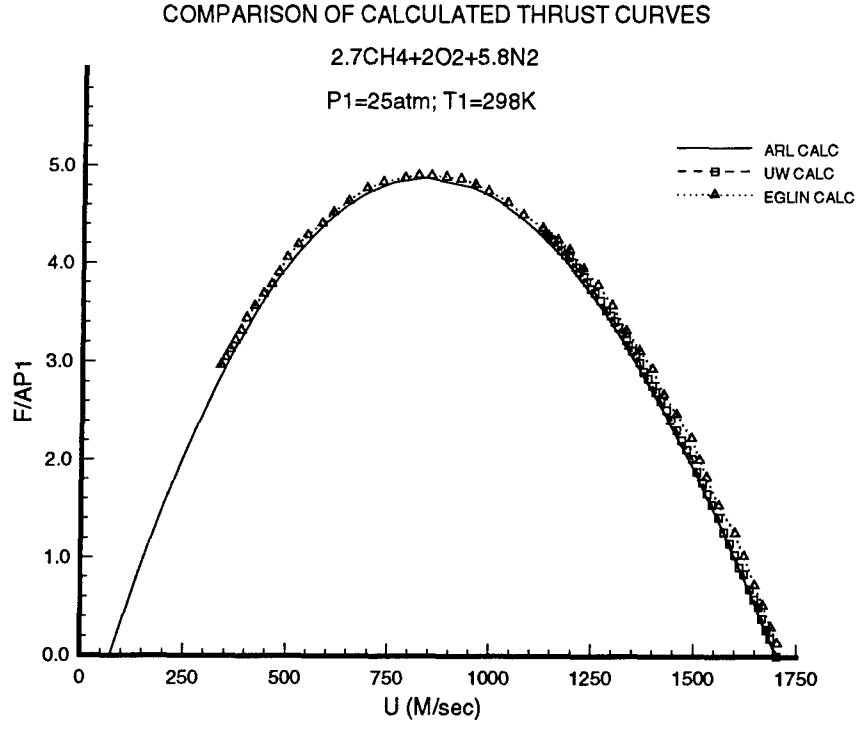

Figure 9: Comparison of calculated thrust curves.

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